The Mirrors Model : Macroscopic Diffusion Without Noise or Chaos

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We consider a discrete version of the mirrors model in a finite d-dimensional domain and connected to particles reservoirs at fixed chemical potentials. The dynamics is purely deterministic and non-ergodic. We study the macroscopic current of particles in the stationary regime. We show first that when the size of the system goes to infinity, the behaviour of the stationary current of particles is governed by the proportion of orbits crossing the system. Using this approach, we show that Fick's law relating the stationary macroscopic current of particles to the concentration difference holds in three dimensions and above. The negative correlations between crossing orbits play a key role in the argument.

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The mirrors model was introduced by Ruijgrok and Cohen [6] as a lattice version of the random Lorentz gas or the Ehrenfest wind-tree model. A central question regarding those models is whether a non-chaotic dynamics may give rise to a *macroscopic* diffusive behaviour. In this respect, the mirrors model is quite spectacular : a quick look at the structure of the orbits reveals its total lack of ergodicity.

It has even been proved [2] that, in any dimension, the motion of a particle in an environment of randomly orientated mirrors is not a gaussian diffusion. More precisely this means that, under a diffusive rescaling of space and time, the law of the position of the particle does not converge to a gaussian distribution. The goal of this Letter is to show that in spite of these unpromising properties, the mirrors models does exhibit normal macroscopic conductive properties when $d \geq 3$. It turns out that quite weak conditions on the statistics of orbits are sufficient to ensure the validity of Fick's law at the macroscopic level. It is therefore not necessary that orbits behave as a Gaussian diffusion to ensure the validity of Fick's law. Thus, the normal *macroscopic* laws of diffusion apply to a much wider class of dynamical systems than generally expected. As we explain below, in a system connected to particles reservoirs, proving Fick's law is equivalent to establishing a law of large number (in the size of the system) for the macroscopic current of particles. Using the reversibility of the dynamics, we show that the number of orbits travelling from one side of the system to the other one basically determines the value of the current in the stationary state, when the system is large. This allows to formulate conditions on the expectation and on the variance of the number of crossing orbits that ensure the validity of Fick's law. This was also the starting point of the analysis of [5] where a rigorous proof is given in the case of an anisotropic version of the random Lorentz gas.

We recall now briefly the set-up of the original mirrors model. Particles travel on the edges of $\mathbb{Z}^2$ with unit speed. Mirrors are located at some vertices of the lattice and take two possible angular orientations : $\{\frac{\pi}{4}, \frac{3\pi}{4}\}$. When a particle hits a mirror, it gets deflected according to the laws of specular reflection, see figure 2 for sample trajectories of particles. It is convenient to think that every particle starts at time zero with a given velocity at a vertex of the lattice $\mathcal{Q}$ that is obtained by taking the middle point of every edge of $\mathbb{Z}^2$. As all particles move with unit velocity, one can simply observe the evolution of the system at discrete times $t \in \mathbb{N}$. At those times, the particles will be always located at one of the vertices of the new lattice $\mathcal{Q}$ with a well-defined velocity. In general, the orientation of the mirrors is picked randomly. It is obvious that the motion of a single particle can not be described as a Markov process. When a particle hits a mirror for the second time, no matter how far back in the past the first visit occurred, its reflection is deterministic, see for instance figure 2.

We come now to a more general definition of the dynamics in d dimensions . We denote by $\mathbf{z} = (z_1, \dots, z_d)$ a generic element of $\mathbb{Z}^d$. As for $\mathbb{Z}^2$, we consider the set of midpoints of edges of an hypercube of $\mathbb{Z}^d$ of side N and with periodic conditions in all but the first direction. We call this set $\mathcal{Q}$. It may be described as follows : $\mathcal{Q} = \bigcup_{i=1}^d L_i$ where $L_i = \{\mathbf{z} + \frac{1}{2}\mathbf{e}_i : \ 0 \leq z_1 \leq N-1, \ (z_2, \dots, z_d) \in (\mathbb{Z}/N\mathbb{Z})^{d-1}\}$. Let $(\mathbf{e}_1, \dots, \mathbf{e}_d)$ the canonical basis of $\mathbb{R}^d$, the space of possible velocities is $\mathcal{P} = \{\pm\frac{\mathbf{e}_1}{2}, \dots, \pm\frac{\mathbf{e}_d}{2}\}$ and the phase space of the dynamics is

$$\mathcal{M} = \{(\mathbf{q}, \mathbf{p}) : \mathbf{q} \in \mathcal{Q}, \mathbf{p} \in \mathcal{P} \text{ s. t. if } \mathbf{q} \in L_i \text{ then } \mathbf{p} = \pm\frac{\mathbf{e}_i}{2}\}.$$

We denote a generic point of $\mathcal{M}$ by $(\mathbf{q}, \mathbf{p})$. The set of points in $\mathcal{M}$ whose spatial coordinate belongs to the boundaries of the system is $B = B_- \cup B_+$, with

$$B_- = \{x = (\mathbf{q}, \mathbf{p}) \in \mathcal{M} : \mathbf{q} = (q_1, \dots, q_d) \in L_1, q_1 = \frac{1}{2}\}$$
$$B_+ = \{x = (\mathbf{q}, \mathbf{p}) \in \mathcal{M} : \mathbf{q} = (q_1, \dots, q_d) \in L_1, q_1 = N - \frac{1}{2}\}.$$

For each $\mathbf{z} \in \mathbb{Z}^d$, we define the action of a "mirror" on the velocity of an incoming particle by $\pi(\mathbf{z}; \cdot)$, a bijection

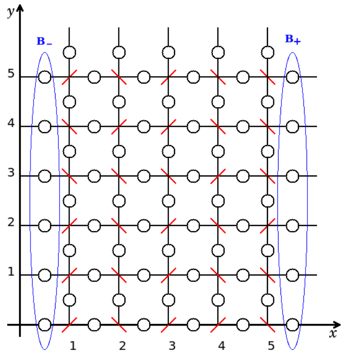

FIG. 1: The spatial component of the phase space $\mathcal{M}$ and of the sets B_- and B_+ in $2D$.

of $\mathcal{P}$ into itself. It satisfies the following conditions :

$$\begin{cases} \pi(\mathbf{z}; -\pi(\mathbf{z};\mathbf{p})) = -\mathbf{p}, \quad \forall \mathbf{z} \in \mathbb{Z}^d, \forall \mathbf{p} \in \mathcal{P} \\ \pi(0, z_2, \ldots, z_d; -\frac{\mathbf{e}_1}{2}) = \frac{\mathbf{e}_1}{2} \\ \pi(N, z_2, \ldots, z_d; \frac{\mathbf{e}_1}{2}) = -\frac{\mathbf{e}_1}{2}, \ (z_2, \ldots, z_d) \in (\mathbb{Z}/N\mathbb{Z})^{d-1} \end{cases} \tag{1}$$

The dynamics is defined on $\mathcal{M}$ in the following way. For any $(\mathbf{q}, \mathbf{p}) \in \mathcal{M}$:

$$F(\mathbf{q}, \mathbf{p}) = (\mathbf{q} + \mathbf{p} + \pi(\mathbf{q} + \mathbf{p}; \mathbf{p}), \pi(\mathbf{q} + \mathbf{p}; \mathbf{p}))\,.$$

It is easy to check that the map F is a bijection on $\mathcal{M}$. The two last conditions in (1) are just saying that when particles hit the boundaries they are reflected backwards. We define an operator $R : \mathcal{M} \to \mathcal{M}$ which reverses the velocities by $R(\mathbf{q}, \mathbf{p}) = (\mathbf{q}, -\mathbf{p})$ and we see that the first of the conditions (1) ensures that the map F is *reversible*, i.e. $F^{-1} = RFR$. We define the orbit of a point $x \in \mathcal{M}$, $\mathcal{O}_x = \{y \in \mathcal{M} : \exists t \geq 0, F^t(x) = y\}$ and its period, $T(x) = \inf\{t \geq 0 : F^t(x) = x\}$. From the fact that F is bijective, one infers that for every $x \in \mathcal{M}$, $\mathcal{O}_x$ is a loop : $T(x) \leq |\mathcal{M}|$ and that orbits are non-intersecting : if $y \notin \mathcal{O}_x$, then $\mathcal{O}_x \cap \mathcal{O}_y = \emptyset$. A given orbit is also non-self-intersecting : if $y \in \mathcal{O}_x$ and $y \neq x$ then $F(y) \neq F(x)$.

As we are interested in the transport of particles, we define occupation variables $\sigma(\mathbf{q}, \mathbf{p}; t) \in \{0, 1\}$ that record the absence or presence of a particle at position $\mathbf{q}$ with velocity $\mathbf{p}$ at time $t \in \mathbb{N}$. When connecting the system to external particles reservoirs, we obtain the following evolution rule : given $\sigma(\cdot; t-1)$, we define $\sigma(\cdot; t)$ for all $t \in \mathbb{N}^*$ by

$$\sigma(x;t) = \begin{cases} \sigma(F^{-1}(x); t-1) & \text{if} \quad x \notin B_- \cup B_+ \\ \sigma_x^-(t-1) & \text{if} \quad x \in B_- \\ \sigma_x^+(t-1) & \text{if} \quad x \in B_+ . \end{cases}$$

The families of random variables $\{\sigma_x^-(t) : x \in B_-, t \in \mathbb{N}\}$ and $\{\sigma_x^+(t) : x \in B_+, t \in \mathbb{N}\}$ consist of independent Bernoulli variables with respective parameters ρ_- and ρ_+. If one chooses $\{\sigma(x;0) : x \in \mathcal{M}\}$ to be a collection of independent random variables, then it is easy to see by induction that at any $t \geq 0$, $\{\sigma(x;t) : x \in \mathcal{M}\}$ is a collection of i.i.d Bernoulli random variables. To simplify a bit the discussion, we choose an homogeneous initial distribution, i.e. all Bernoulli random variables have a common parameter ρ_I. The distribution of the collection $\{\sigma(x;t) : x \in \mathcal{M}\}$ becomes stationary after a *finite* time. More precisely, for any $t \geq |\mathcal{M}|$, we have the following equality in law :

$$\sigma(x,t) = \begin{cases} \sigma_I & \text{if} \quad \mathcal{O}(x) \cap B = \emptyset \\ \sigma_- & \text{if} \quad F^{-t^*}(x) \in B_- \\ \sigma_+ & \text{if} \quad F^{-t^*}(x) \in B_+ \end{cases}$$

where $t^* = \inf\{t : F^{-t}(x) \in B\}$ and $\sigma_\pm$ and σ_I are Bernoulli random variables of parameter $\rho_\pm$ and ρ_I.

Proceeding as in [5], it is possible to show that when the size of the system goes to infinity, the stationary current converges in probability to the proportion of crossing orbits times the chemical potentials difference. We define the average current of particles that crosses the hyperplane $\mathcal{Q}^l = \{\mathbf{q} \in \mathcal{Q} : q_1 = l + \frac{1}{2}\}$, $l \in \{1, \ldots, N-2\}$ during a diffusive time interval N^2 as a function of a configuration $\sigma \in \{0,1\}^{\mathcal{M}}$:

$$J(l,t) = \frac{1}{N^{d+1}} \sum_{s=t}^{t+N^2} \sum_{x \in \mathcal{M}} \sigma(x;s) \Delta(x,l) \tag{2}$$

where $\Delta(x,l) = 2(\mathbf{p} \cdot \mathbf{e}_1) \mathbf{1}_{\mathbf{q} \in \mathcal{Q}^l}$,with $x = (\mathbf{q}, \mathbf{p})$. Thus $\Delta(x,l)$ takes the value $+1$ (resp. -1) if x crosses the slice $\mathcal{Q}^l$ from left to right (resp. from right to left). We denote by $\mathcal{N}_\pm$ the numbers of crossings from $B_\pm$ to $B_\mp$ induced by F, i.e. $\mathcal{N}_\pm = |S_\pm|$ where $S_\pm$ is given by

$$S_\pm = \{x \in B_\pm : \exists s > 0, \forall 0 < j < s, \ F^j(x) \notin B_\pm, F^s(x) \in B_\mp\}. \tag{3}$$

One notes that $\mathcal{N}_+ = \mathcal{N}_-$. Indeed, since every orbit is closed, it must contain as many left-to-right than

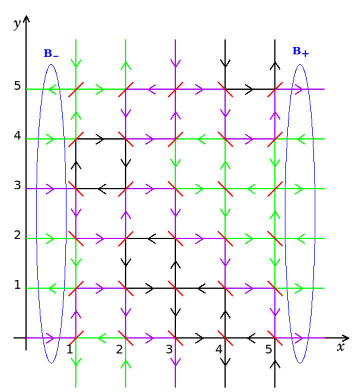

FIG. 2: $N = 6$. Crossing orbits are coloured in purple, internal loops in black and non-crossing orbits are coloured in green. The travel direction given by the arrows is arbitrary. Each edge of the crossing orbits will be used twice in a given orbit : once in each direction. For this configuration of mirrors $\mathcal{N} = 2$.

right-to-left crossings. Thus, we set $\mathcal{N} = \mathcal{N}_+ = \mathcal{N}_-$. Proceeding as in [5], we get that for any $t \geq |\mathcal{M}|$, $\mathbb{E}[J(l,t)] = \frac{\mathcal{N}}{N^{d-1}}(\rho_- - \rho_+)$. This relation implies that the average current flows in the "right" direction and that when $\rho_- \neq \rho_+$, the average current in the stationary state is different from 0 if and only if $\mathcal{N} \neq 0$. Moreover, for every $\delta > 0$, any $t \geq |\mathcal{M}|$ and $l \in \{1, \ldots, N-2\}$,

$$\mathbb{P}\left[\left|J(l,t) - \frac{\mathcal{N}}{N^{d-1}}(\rho_- - \rho_+)\right| \geq \delta\right] \leq 2\exp(-\delta^2 N^{d+1}). \tag{4}$$

We take now random configurations of reflectors $\{\pi(\mathbf{z};\cdot) : \mathbf{z} \in \mathbb{Z}^d\}$. The law of the reflectors is denoted by $\mathbb{Q}$. The map F becomes now a random map. The model satisfies *Fick's law* if and only if there exists some $\kappa > 0$ (the conductivity) such that $\forall \epsilon > 0$,

$$\lim_{N\to\infty} \lim_{t\to\infty} \mathbb{P} \times \mathbb{Q}[|NJ(l,t) - \kappa(\rho_- - \rho_+)| > \epsilon] = 0. \tag{5}$$

As in [5], it is easy to infer from (4) that this holds if and only if there exists $\kappa > 0$ such that for any $\epsilon > 0$,

$$\lim_{N\to\infty} \mathbb{Q}\left[\left|\frac{\mathcal{N}}{N^{d-2}} - \kappa\right| > \epsilon\right] = 0. \tag{6}$$

We see that the central object to study is the distribution of the number of crossing orbits $\mathcal{N}$. The expectation of this quantity is related to the probability that one orbit crosses the system, while the variance is given in terms of the joint probability that orbits with two different starting points cross the system. Indeed by periodicity, we have, using the notation $O = ((\frac{1}{2}, 0, \ldots, 0), \frac{\mathbf{e}_1}{2})$:

$$\mathbb{E}\left[\frac{\mathcal{N}}{N^{d-2}}\right] = \frac{N}{N^{d-1}} \sum_{x \in B_-} \mathbb{E}[\mathbf{1}_{x\in S}] = N\mathbb{Q}[O \in S] \tag{7}$$

and

$$\mathrm{Var}\left[\frac{\mathcal{N}}{N^{d-2}}\right] = \frac{1}{N^{2d-4}} \sum_{x,y \in B_-} \delta(x,y) = \frac{1}{N^{d-3}} \sum_{x \in B_-} \delta(O,x) \tag{8}$$

with $\delta(x,y) = \mathbb{Q}[x \in S, y \in S] - \mathbb{Q}[x \in S]\mathbb{Q}[y \in S]$.

Thus if the two following **Crossing Conditions** *are satisfied :*

1. *There exist $\kappa > 0$ such that the RHS of (7) converges to κ as $N \to \infty$.*
2. *The RHS of (8) goes to zero as $N \to \infty$.*

then Fick's law (5) holds in the stationary state. We note first that when $d = 2$, (6) can not hold, whatever the distribution $\mathbb{Q}$ is. To see this, we adapt an argument found in [4]. Indeed the spatial part of each crossing orbit crosses any "vertical" section $\mathcal{Q}^l$ an odd number of times. On the other hand, the spatial part of any non-crossing orbit must cross any vertical section an even number of times, see Figure 2. Thus, N and $\mathcal{N}$ must have the same parity. This implies that there can not exists $\kappa > 0$ such that (6) holds when $d = 2$. The origin of this issue lies in the strong correlations between crossing orbits that are present in two dimensions.

We turn now to the higher dimensional case $d \geq 3$ equipped with some natural distribution $\mathbb{Q}$. Now observe that if $\mathbb{Q}[\pi(\mathbf{z}; \frac{e_i}{2}) = -\frac{e_i}{2}] > 0$ for some $i = 1, \ldots, d$ then an orbit starting from O will encounter this type of reflecting mirror after an exponential number of steps and therefore $\mathbb{Q}[0 \in S] \leq e^{-cN}$ for some $c > 0$. This, in turn, implies that $\lim_{N\to\infty} N\mathbb{Q}[0 \in S] = 0$ and that Fick's law can not hold. Thus from now on, we consider maps such that $\pi(\mathbf{z}; \frac{e_i}{2}) \neq -\frac{e_i}{2}$ if $0 < z_1 < N$ and such that the conditions (1) are satisfied. We call the set of such maps Π. We take $\mathbb{Q}$ such that the collection of maps

$$\{\pi(\mathbf{z}; .) : 0 < z_1 < N,\ (z_2, \ldots, z_d) \in (\mathbb{Z}/N\mathbb{Z})^{d-1}\}$$

is independent and that each map is uniformly distributed over Π. We note first that if the law of an orbit with respect to $\mathbb{Q}$ was similar to the law of a simple random walk, then there would be a $\kappa > 0$ such that $\lim_{N\to\infty} N\mathbb{Q}[0 \in S] = \kappa$, this follows from the gambler's ruin argument. Similarly, if the orbits were independent objects, then the RHS of (8) would go to zero because the only non-zero term would be the one with $x = O$ and $\mathbb{Q}[O \in S] \sim \kappa/N$. We also note that the average stationary current is identified as the difference between chemical potentials times the probability that a particle crosses the system, an idea that was put forward in [3], in the context of chaotic systems. The law $\mathbb{Q}$ of the mirrors induces a law on the set of orbits which is a priori very far from the distribution of independent simple random walks. The set of orbits is a very interesting lattice object in itself which features some (self-)avoiding properties as we mentioned above.

Fortunately, what is needed to ensure the validity of (6) is much less than the full joint distribution of the orbits. Thanks to (7) and (8), one only has to analyze the marginal of a path starting on the boundary and also the joint probability of two such paths. The distribution of a path starting at O (i.e. on the boundary) is similar to the the one of a "true" self-avoiding random walk [1] but defined on $\mathcal{Q}$ rather than on $\mathbb{Z}^d$ and with further constraints. The diffusive behaviour of those walks for $d \geq 3$ has been conjectured in [1], see also the rigorous results of [7]. It can be expected that as the dimensionality of the system increases, the effect of the revisits of an orbit to the same mirror decreases. In a process where the mirrors are flipped randomly after being used (i.e memory effects are killed), we computed that in $d = 3$ the crossing probability is $\sim 3/2N$. Numerical simulations in $d = 3$ show that this number is indeed a good approximation. The log log plot of the crossing probability

$\mathbb{Q}[O \in S]$ is given in figure 3 for N up to 400. The corresponding conductivity is $\kappa = 1.535 \pm 0.005$. As the conductivity measured in simulations is slightly higher than $3/2$, it indicates that recollisions tend to push forward the orbit.

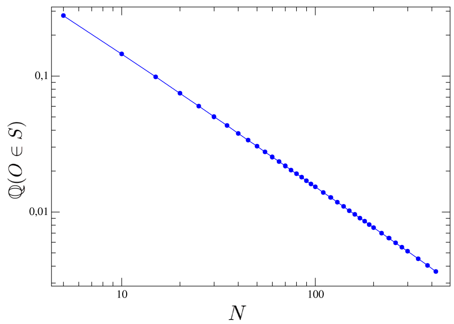

FIG. 3: $\mathbb{Q}(O \in S)$ for N from 5 to 420. The 95% confidence interval is about half the size of a dot.

We must show now that $\sum_{x \in B_-} \delta(O,x) \to 0$ as $N \to \infty$. We know that this sum is positive because it is a variance, and thus it is enough to get an upper bound on the sum. In order to do this, we show that for most $x \in B_-$, $\delta(O,x) < 0$. Given an orbit $\mathcal{O}$, we denote by $\gamma(\mathcal{O})$ the set of edges of $\mathbb{Z}^d$ used by $\mathcal{O}$. Two *crossing orbits* $\mathcal{O}$ and $\mathcal{O}'$ are incompatible if $\gamma(\mathcal{O}) \cap \gamma(\mathcal{O}') \neq \emptyset$ and compatible otherwise. If $\mathbb{Q}(\mathcal{O}_1, \mathcal{O}_2)$ is the joint probability of two orbits $\mathcal{O}_1$ and $\mathcal{O}_2$ then $\mathbb{Q}(\mathcal{O}_1, \mathcal{O}_2) = 0$ when $\mathcal{O}_1$ and $\mathcal{O}_2$ are incompatible. If they do not share any mirrors, then $\mathbb{Q}(\mathcal{O}_1, \mathcal{O}_2) = \mathbb{Q}(\mathcal{O}_1)\mathbb{Q}\mathcal{O}_2)$. From those two properties, we obtain that for $x \in B_-$,

$$\begin{aligned} \delta(O,x) &= \sum_{\mathcal{O}_0,\mathcal{O}_x} \left(\mathbb{Q}(\mathcal{O}_0,\mathcal{O}_x) - \mathbb{Q}(\mathcal{O}_0)\mathbb{Q}(\mathcal{O}_x)\right) \\ &\quad - \sum_{\mathcal{O}_0,\mathcal{O}_x}{}' \mathbb{Q}(\mathcal{O}_0)\mathbb{Q}(\mathcal{O}_x). \end{aligned} \tag{9}$$

Both sums run over orbits that cross the box $\mathcal{Q}$. The first sum runs over compatible orbits such that $\gamma(\mathcal{O}_0)$ and $\gamma(\mathcal{O}_x)$ share a vertex of $\mathbb{Z}^d$ where a mirror sits. The second (prime) sum runs over *incompatible* orbits $\mathcal{O}_0, \mathcal{O}_x$.

Correlations are created from two opposite origins, corresponding to each of the two sums. If two orbits $\mathcal{O}_1$ and $\mathcal{O}_2$ share some mirrors, then it is easy to see that $\mathbb{Q}(\mathcal{O}_1, \mathcal{O}_2) > \mathbb{Q}(\mathcal{O}_1)\mathbb{Q}(\mathcal{O}_2)$ implying that the first sum is strictly positive. This is a "cooperative" effect, the orbits help each other crossing the system. The second sum corresponds to a *jamming* effect : an orbit starting from O and crossing the system occupies a certain number of horizontal edges. Because distinct orbits can not share the same edges, the occupied edges are no more available for an orbit starting from $x \in B_-$, this creates negative correlations. Numerical simulations in $d = 3$ show that the latter effect dominates. For all but a few points within confidence intervals, the correlations $\delta(O,x)$ for $x \neq O$ are not only small but negative, see figure 4. The only exceptions are points $((1/2,1,0), \frac{\mathbf{e}_1}{2})$, $((1/2,0,1), \frac{\mathbf{e}_1}{2})$, $((1/2,N-1,0), \frac{\mathbf{e}_1}{2})$ and $((1/2,0,N-1), \frac{\mathbf{e}_1}{2})$ which give clearly positive correlations. However, we checked that for $N = 70$ $\sum_{y=1}^{N-1} \delta(O, ((1/2,y,0), \frac{\mathbf{e}_1}{2})) = -1.360 \times 10^{-04} \pm 1.47 \times 10^{-05}$, i.e. it is negative with a margin of more than 9σ. $\sum_{z=1}^{N-1} \delta(O, ((1/2,0,z), \frac{\mathbf{e}_1}{2}))$ must be equal by symmetry. Increasing values of N do not modify this behaviour. Since we know already that $\mathbb{Q}[O \in S] \sim \kappa/N$, as $N \to \infty$, we conclude with the same margin that $\sum_{x \in B_-} \delta(O,x) \leq \kappa/N \to 0$, as $N \to \infty$. We expect

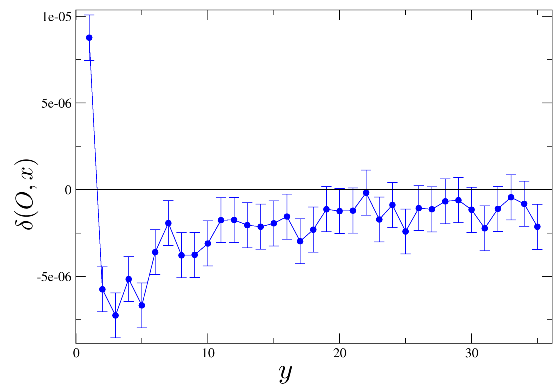

FIG. 4: $\delta(O,x)$ for $x = ((1/2,y,0), \frac{\mathbf{e}_1}{2})$. N=70. We draw the 95% confidence interval.

the same behaviour in $d \geq 3$. A rigorous proof that the *crossing conditions* introduced above are satisfied seems to be within reach in the present model. Moreover, it is possible to draw a general conclusion from the above discussion. If one is really interested in deriving macroscopic laws from microscopic dynamics, many detailed properties of the latter are irrelevant. What is required are much weaker properties than chaoticity, ergodicity or Gaussian behaviour of the orbits. In the present context, the minimal properties necessary to obtain Fick's law are encapsulated in the crossing conditions. It is of course natural to seek similar weak conditions in different contexts as for instance in the problem of the derivation of Fourier's law.

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